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# Supporting Information



## Ni→B Interactions in Nickel Phosphino-Alkynyl-Borane Complexes

**Xiaoxi Zhao, Edwin Otten, Datong Song, and Douglas W. Stephan*[a]**

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## Experimental Methods

### General Considerations

All preparations and manipulations were performed on a double manifold $N_2$/vacuum line with Schlenk-type glassware or in a $N_2$-filled M-Braun glove box. Solvents (Aldrich) were dried using an Innovative Technologies solvent system. NMR spectra were obtained on a Bruker Avance 400 MHz spectrometer and spectra were referenced to residual solvent ($^1$H, $^{13}$C) or externally ($^{11}$B; $BF_3OEt_2$, $^{19}$F; $CFCl_3$, $^{31}$P; 85% $H_3PO_4$). NMR solvents were purchased from Cambridge Isotopes, dried over $CaH_2$ or Na/benzophenone, vacuum distilled prior to use and stored over 4Å molecular sieves in the glovebox. IR spectra were recorded on a Perkin-Elmer Spectrum One FT-IR spectrometer. $B(C_6F_5)_3$ was generously provided by Nova Chemicals. Combustion analysis was performed in house on a Perkin-Elmer CHN Analyzer.

**Synthesis of *t*Bu$_2$PHC=CBCl(C$_6$F$_5$)$_2$ 1** To a solution of $ClB(C_6F_5)_2$ (733 mg, 1.93 mmol) in toluene (2 mL) was added a solution of HCCP*t*Bu$_2$ (328 mg, 1.93 mmol) in toluene (8 mL) at -35 $^o$C. The reaction was stirred for 1 h, during which time the solution color turned yellow. After the solvent was completely pumped off, pentane (12 mL) was added and the mixture was stirred until an off-white solid formed. The supernatant liquid was decanted and the solid product was washed with pentane. Drying *in vacuo* afforded an off-white powder. This product was used in the subsequent reactions without further purification. Yield: 761 mg, 72%. $^1$H NMR: 5.80 (d, 1H, $^1J_{HP}$ = 469 Hz, P*H*), 1.51 (d, 18H, $^3J_{HP}$ = 18.8 Hz, *t*Bu). $^{11}$B{$^1$H} NMR: -12.80 (s). $^{13}$C{$^1$H} NMR: 148.26 (dm, $^1J_{CF}$ = 243 Hz, *o*-$C_6F_5$), 145.18 (br, C=*C*B), 140.07 (dm, $^1J_{CF}$ = 251 Hz, *p*-$C_6F_5$), 137.57 (dm, $^1J_{CF}$ = 248 Hz, *m*-$C_6F_5$), 119.81 (br, quat-$C_6F_5$), 67.43 (d, $^1J_{CP}$ = 155 Hz, C=*C*P), 35.41 (d, $^1J_{CP}$ = 42 Hz, quat-*t*Bu), 26.99 (d, $^2J_{CP}$ = 2.5 Hz, *t*Bu). $^{19}$F NMR: -133.09 (m, 4F, *o*-$C_6F_5$), -160.50 (t, 2F, $^3J_{FF}$ = 20 Hz, *p*-$C_6F_5$), -166.08 (m, 4F, *m*-$C_6F_5$). $^{31}$P {$^1$H} NMR: 25.50 (s). Anal. Calcd. for $C_{22}H_{19}BClF_{10}P$: C, 47.99; H, 3.48. Found: C, 47.87; H, 3.80 %.

**Synthesis of *t*Bu$_2$PHC=CBH(C$_6$F$_5$)$_2$ 2** Compound **1** (368 mg, 0.668 mmol) was stirred with $Me_2SiHCl$ (1.0 g, 5.83 mmol) overnight in $CH_2Cl_2$. After confirming full conversion to the product by NMR of the reaction mixture, all the volatiles were completely pumped off. The residue was dissolved in toluene and passed through neutral alumina to eliminate high molecular weight impurities. The filtrate was dried and the product was recrystallized by layering $CH_2Cl_2$ solution with pentane at RT overnight. The product colorless crystals were separated from the supernatant, from which more product was recrystallized using $CH_2Cl_2$/pentane. The combined product was dried in vacuo. Yield: 273 mg, 79%. Single crystals suitable for X-ray diffraction were grown by layering a $CH_2Cl_2$ solution of the product with pentane at 25$^o$C. $^1$H NMR: 5.70 (dd, 1H, $^1J_{HP}$ = 464 Hz, $^5J_{HH}$ = 2.0 Hz, P*H*), 3.25 (q, 1H, $^1J_{HB}$ = 91 Hz, B*H*), 1.48 (d, 18H, $^3J_{HP}$ = 18.8 Hz, *t*Bu). $^{11}$B{$^1$H}: -29.15 (s). $^{13}$C{$^1$H} NMR: 147.98 (dm, $^1J_{CF}$ = 235 Hz, *o*-$C_6F_5$), 138.77 (dm, $^1J_{CF}$ = 245 Hz, *p*-$C_6F_5$), 136.93 (dm, $^1J_{CF}$ = 261 Hz, *m*-$C_6F_5$), 120.90 (br, quat-$C_6F_5$), 64.37 (d, $^1J_{CP}$ = 158 Hz, C=*C*P), 34.72 (d, $^1J_{CP}$ = 44 Hz, quat-*t*Bu), 26.70 (d, $^2J_{CP}$ = 2.6 Hz, *t*Bu). C=*C*B was not observed. $^{19}$F NMR: -133.23 (dm, 4F, $^3J_{FF}$ = 21 Hz, *o*-$C_6F_5$), -162.79 (t, 2F, $^3J_{FF}$ = 20 Hz, *p*-$C_6F_5$), -166.67 (m, 4F, *m*-$C_6F_5$). $^{31}$P{$^1$H} NMR : 24.18 (s). IR ($CH_2Cl_2$, cm$^{-1}$): 2125

(?(C=C)). Anal. Calcd. for $C_{22}H_{20}BF_{10}P$: C, 51.19; H, 3.91. Found: C, 51.35; H, 4.02 %.

**Synthesis of ($t$Bu$_2$PC=CB(C$_6$F$_5$)$_2$)Ni(COD)·0.5C$_7$H$_8$ 4** This compounds was obtained in via two synthetic routes. Method 1: To a toluene (1.0 mL) solution of **2** (100 mg, 0.19 mmol) was added a mixture of $B(C_6F_5)_3$ (99 mg, 0.19 mmol) and P$t$Bu$_3$ (39 mg, 0.19 mmol) dissolved in toluene (2.0 mL) at RT. The reaction mixture immediately turned orange-yellow, and became cloudy upon stirring for 1 h. Hexanes (10 mL) were added, and the reaction was left standing at -35$^o$C for 3 h. The mixture was then filtered through Celite and washed with cold hexanes. Upon addition of the combined filtrate to a mixture of $Ni(COD)_2$ (50 mg, 0.18 mmol) and 1,5-cyclooctadiene (190 mg, 1.8 mmol), the reaction immediately started to turn orange, and became red in 15 min. After 6 h of stirring, the solution was pumped down and some toluene was added to dissolve all the red precipitate. The mixture was then filtered through Celite to eliminate small amount of Ni metal that precipitated out of the reaction. The filtrate was further pumped down until a red precipitate started to form. Upon addition of pentane (8 mL) and cooling at -35 $^o$C overnight, the supernatant liquid was removed to afford an orange-red fine crystalline product, which was washed with pentane and dried *in vacuo*. The isolated product was stored at -35 $^o$C to avoid decomposition. Yield: 86 mg, 65 %.

Method 2: **2** (100 mg, 0.19 mmol), $Ni(COD)_2$ (53 mg, 0.19 mmol) and 1,5-cyclooctadiene (210 mg, 1.9 mmol) were mixed together in toluene (5 mL). The initially yellow solution turned deep red upon overnight stirring at RT. The reaction work up was the same as method 1. Yield: 101 mg, 72 %. The crystalline product was suitable for X-ray diffraction. $^1$H NMR ($C_6D_6$): 7.13 (m, 1.5H, *o/p*-Ph, toluene), 7.02 (m, 1H, *m*-Ph, toluene), 5.50 (br, 2H, =C*H*, cod), 4.88 (br, 2H, =C*H*, cod), 2.11 (s, 1.5H, C*H*$_3$, toluene), 1.90 (m, 4H, C*H*$_2$, cod), 1.67 (m, 4H, C*H*$_2$, cod), 1.22 (d, 18H, $^3J_{HP}$ = 12.3 Hz, *t*Bu). $^{11}$B{$^1$H} NMR ($C_6D_6$): 6.98 (br). $^{13}$C{$^1$H} NMR ($C_6D_6$): 147.89 (dm, $^1J_{CF}$ = 241 Hz, *o*-C$_6$F$_5$), 140.49 (dm, $^1J_{CF}$ = 247 Hz, *p*-C$_6$F$_5$), 137.96 (dm, $^1J_{CF}$ = 250 Hz, *m*-C$_6$F$_5$), 137.90 (s, *i*-Ph, toluene), 129.34 (s, *o*-Ph, toluene), 128.69 (s, *m*-Ph, toluene), 125.68 (s, *p*-Ph, toluene), 120.70 (d, $^1J_{CP}$ = 57 Hz, C=*C*P), 108.62 (d, $^3J_{CP}$ = 11.2 Hz, =*C*H, cod), 98.70 (s, =*C*H, cod), 33.03 (d, $^1J_{CP}$ = 25 Hz, quat-*t*Bu), 31.03 (s, $CH_2$, cod), 29.60 (d, $^2J_{CP}$ = 14 Hz, *t*Bu), 28.31 (s, $CH_2$, cod), 21.42 (s, *C*H$_3$, toluene). C=*C*B and quat-C$_6$F$_5$ carbons were not observed. $^{19}$F NMR ($C_6D_6$): -129.32 (m, 4F, *o*-C$_6$F$_5$), -154.85 (t, 2F, $^3J_{FF}$ = 21Hz, *p*-C$_6$F$_5$), 163.13 (m, 4F, *m*-C$_6$F$_5$). $^{31}$P{$^1$H} NMR ($C_6D_6$): 6.86 (s). IR (thin film from $CH_2Cl_2$, cm$^{-1}$): 1881 (?(C=C)). Anal. Calcd. for $C_{30}H_{30}BF_{10}PNi{\cdot}C_{3.5}H_4$: C, 55.34; H, 4.71. Found: C, 55.35; H, 5.00 %.

**Synthesis of [($t$Bu$_2$PC=CB(C$_6$F$_5$)$_2$)Ni(NCMe)]$_2$ 5** Compound **4** (24 mg, 0.033mmol) and acetonitrile (50 µL, 0.96 mmol) were mixed in benzene (2 mL). Dark brown crystals formed out of the reaction mixture overnight at RT. The crystals were isolated and washed with benzene (2 x 1 mL) and pentane (2 mL). Yield: 9 mg, 45 %. The crystalline poduct was suitable for X-ray diffraction. $^1$H NMR (THF-d$_8$): 2.52 (br), 2.18 (s), 1.28 (br,m). $^{11}$B{$^1$H} NMR (THF-d$_8$): no signal was observed. $^{19}$F NMR (THF-d$_8$): -130.33 (m, 8F, *o*-C$_6$F$_5$), -159.68 (t, 4F, $^3J_{FF}$ = 20Hz, *p*-C$_6$F$_5$), -165.97 (m, 8F, *m*-C$_6$F$_5$). $^{31}$P{$^1$H} NMR (THF-d$_8$): 53.16 (s). IR

(KBr, $cm^{-1}$): 2269 (?(N=C)), 1838 (?(C=C)). Anal. Calcd. for $C_{48}H_{42}B_2F_{20}N_2P_2Ni_2$: C, 46.96; H, 3.45; N, 2.28. Found: C, 47.22; H, 3.51; N, 2.82 %.

***Computational Methods***

DFT calculations were performed using Gaussian 03.[(ref)] Geometry optimization was carried out using the B3PW91 method[(ref)] and 6-311G** basis set implemented in Gaussian 03 software. Frequency analysis performed after geometry optimization confirmed that no imaginary frequency was present.

Optimized atomic coordinates for **$3_{calc}$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 15 | 0 | 0.597677 | 8.859701 | 5.585688 |
| 2 | 9 | 0 | -0.178444 | 5.680712 | 2.408723 |
| 3 | 9 | 0 | 2.370649 | 4.820945 | 7.374146 |
| 4 | 9 | 0 | -0.172882 | 1.959481 | 4.589355 |
| 5 | 9 | 0 | 2.944153 | 2.418310 | 3.828907 |
| 6 | 9 | 0 | -0.348069 | 0.191678 | 6.591622 |
| 7 | 9 | 0 | 3.348418 | 1.716938 | 1.277529 |
| 8 | 9 | 0 | 2.183798 | 3.036807 | 9.355262 |
| 9 | 9 | 0 | 0.828574 | 0.715547 | 8.981047 |
| 10 | 9 | 0 | 0.243404 | 4.960117 | -0.130367 |
| 11 | 9 | 0 | 2.003572 | 2.978959 | -0.714079 |
| 12 | 6 | 0 | 0.938422 | 7.175646 | 5.301282 |
| 13 | 6 | 0 | 1.367017 | 4.083592 | 3.233408 |
| 14 | 6 | 0 | 0.429750 | 2.257267 | 5.745054 |
| 15 | 6 | 0 | 1.035921 | 5.978360 | 5.046246 |
| 16 | 6 | 0 | 1.104417 | 3.470817 | 5.892235 |
| 17 | 6 | 0 | 0.903654 | 4.348163 | 0.850086 |
| 18 | 6 | 0 | 0.320082 | 1.328737 | 6.768139 |
| 19 | 6 | 0 | 0.707022 | 4.709987 | 2.174109 |
| 20 | 6 | 0 | 2.251435 | 3.061630 | 2.882975 |
| 21 | 6 | 0 | 1.682281 | 3.699650 | 7.142266 |
| 22 | 6 | 0 | 2.482711 | 2.684542 | 1.569575 |
| 23 | 6 | 0 | 2.999277 | 9.091586 | 3.959790 |
| 24 | 1 | 0 | 3.458470 | 9.575229 | 3.089070 |
| 25 | 1 | 0 | 2.950423 | 8.018770 | 3.760186 |
| 26 | 1 | 0 | 3.661477 | 9.249542 | 4.811993 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 6 | 0 | 0.917176 | 1.595909 | 7.992849 |
| 28 | 6 | 0 | 1.308569 | 9.148497 | 7.330269 |
| 29 | 6 | 0 | 1.799441 | 3.331340 | 0.548413 |
| 30 | 6 | 0 | 1.605539 | 2.786657 | 8.182579 |
| 31 | 6 | 0 | 1.604805 | 9.679875 | 4.184874 |
| 32 | 5 | 0 | 1.166988 | 4.527266 | 4.729267 |
| 33 | 6 | 0 | 1.697576 | 11.185389 | 4.453670 |
| 34 | 1 | 0 | 2.093778 | 11.684909 | 3.562474 |
| 35 | 1 | 0 | 2.372992 | 11.414676 | 5.281548 |
| 36 | 1 | 0 | 0.719315 | 11.625004 | 4.670835 |
| 37 | 6 | 0 | 0.747797 | 9.442025 | 2.931375 |
| 38 | 1 | 0 | 1.248849 | 9.883222 | 2.062125 |
| 39 | 1 | 0 | -0.239971 | 9.901628 | 3.024093 |
| 40 | 1 | 0 | 0.608792 | 8.376249 | 2.732156 |
| 41 | 6 | 0 | 0.851339 | 10.540277 | 7.790359 |
| 42 | 1 | 0 | 1.143621 | 10.686482 | 8.836143 |
| 43 | 1 | 0 | -0.235711 | 10.644330 | 7.728680 |
| 44 | 1 | 0 | 1.303312 | 11.345669 | 7.208335 |
| 45 | 6 | 0 | 0.631801 | 8.096115 | 8.220931 |
| 46 | 1 | 0 | 0.883686 | 8.303210 | 9.267225 |
| 47 | 1 | 0 | 0.971910 | 7.086694 | 7.984029 |
| 48 | 1 | 0 | -0.458144 | 8.124774 | 8.128075 |
| 49 | 6 | 0 | 2.827567 | 9.016907 | 7.446028 |
| 50 | 1 | 0 | 3.120194 | 9.110413 | 8.499023 |
| 51 | 1 | 0 | 3.351742 | 9.801057 | 6.894295 |
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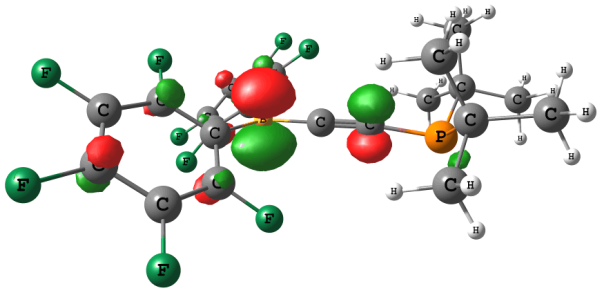
LUMO for **3**$_{calc}$



Optimized Coordinates For **4**$_{calc}$

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
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| 1 | 28 | 0 | -1.341268 | 5.711959 | 4.899160 |
| 2 | 15 | 0 | -0.038203 | 8.898303 | 5.242692 |
| 3 | 9 | 0 | -0.345384 | 5.486743 | 2.161535 |
| 4 | 9 | 0 | 1.642663 | 5.084433 | 7.514333 |
| 5 | 9 | 0 | 0.098536 | 1.717551 | 4.558929 |
| 6 | 9 | 0 | 2.988001 | 2.760760 | 4.149430 |
| 7 | 9 | 0 | 0.230477 | -0.063235 | 6.546818 |
| 8 | 9 | 0 | 3.886222 | 2.125777 | 1.725436 |
| 9 | 9 | 0 | 1.755507 | 3.288996 | 9.477144 |
| 10 | 9 | 0 | 1.053489 | 0.702609 | 9.024365 |
| 11 | 9 | 0 | 0.577094 | 4.836167 | -0.239390 |
| 12 | 9 | 0 | 2.700441 | 3.149245 | -0.498787 |
| 13 | 6 | 0 | 0.022527 | 7.106451 | 5.096431 |
| 14 | 6 | 0 | 1.253715 | 4.131200 | 3.286608 |
| 15 | 6 | 0 | 0.516298 | 2.149569 | 5.760547 |
| 16 | 6 | 0 | 0.625050 | 5.993554 | 5.027455 |
| 17 | 6 | 0 | 0.855110 | 3.490947 | 5.939023 |
| 18 | 6 | 0 | 1.161781 | 4.323785 | 0.844471 |
| 19 | 6 | 0 | -2.512803 | 4.076715 | 5.483326 |
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| 21 | 6 | 0 | 0.574970 | 1.204109 | 6.772483 |
| 22 | 6 | 0 | 0.701759 | 4.641377 | 2.113548 |
| 23 | 6 | 0 | -2.334468 | 4.028985 | 4.119982 |
| 24 | 1 | 0 | -1.549455 | 3.378169 | 3.745929 |
| 25 | 6 | 0 | 2.343547 | 3.279898 | 3.095898 |
| 26 | 6 | 0 | 1.272730 | 3.830620 | 7.225825 |
| 27 | 6 | 0 | 2.838879 | 2.940384 | 1.844900 |
| 28 | 6 | 0 | 2.320641 | 8.609727 | 3.517203 |
| 29 | 1 | 0 | 2.757888 | 8.889689 | 2.550915 |
| 30 | 1 | 0 | 2.143762 | 7.532477 | 3.504896 |
| 31 | 1 | 0 | 3.063252 | 8.822501 | 4.286688 |
| 32 | 6 | 0 | 0.993857 | 1.591532 | 8.037433 |
| 33 | 6 | 0 | 0.887994 | 9.154423 | 6.896717 |
| 34 | 6 | 0 | 2.240805 | 3.463881 | 0.708458 |
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| 38 | 1 | 0 | -2.574417 | 7.612395 | 3.705293 |
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| 44 | 1 | 0 | -3.920950 | 3.915428 | 7.076055 |

| | | | | | |
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| 46 | 1 | 0 | 1.716581 | 11.238046 | 2.848994 |
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| 52 | 6 | 0 | -3.666939 | 6.013581 | 6.628904 |
| 53 | 1 | 0 | -3.117945 | 6.070989 | 7.574127 |
| 54 | 1 | 0 | -4.666155 | 6.422242 | 6.833478 |
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| 56 | 1 | 0 | 0.588053 | 9.463017 | 1.607902 |
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| 59 | 6 | 0 | -3.292428 | 4.554522 | 3.083123 |
| 60 | 1 | 0 | -2.728097 | 4.696601 | 2.158725 |
| 61 | 1 | 0 | -4.060304 | 3.800591 | 2.861233 |
| 62 | 6 | 0 | 0.780726 | 10.642610 | 7.258922 |
| 63 | 1 | 0 | 1.176309 | 10.797636 | 8.269504 |
| 64 | 1 | 0 | -0.259076 | 10.982687 | 7.249890 |
| 65 | 1 | 0 | 1.351800 | 11.281792 | 6.583046 |
| 66 | 6 | 0 | 0.084858 | 8.353955 | 7.933894 |
| 67 | 1 | 0 | 0.483553 | 8.562499 | 8.933429 |
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| 69 | 1 | 0 | -0.971984 | 8.640423 | 7.934692 |
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| 71 | 1 | 0 | 2.723776 | 8.753499 | 7.954660 |
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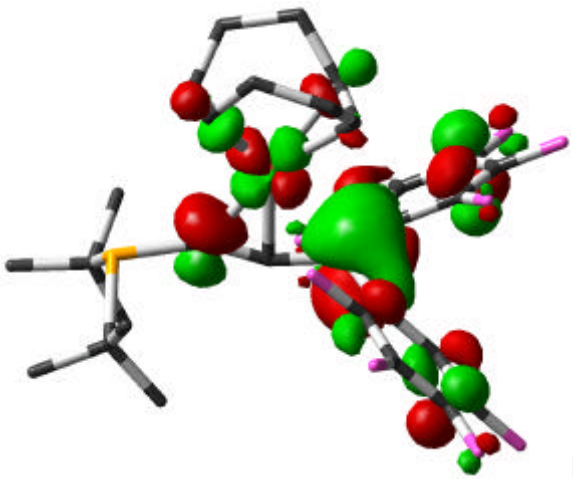

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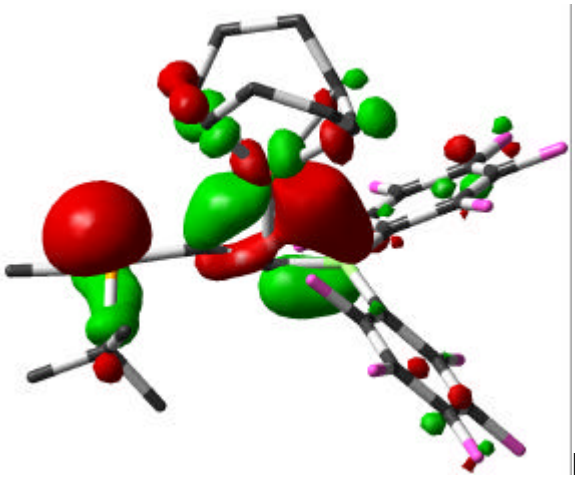

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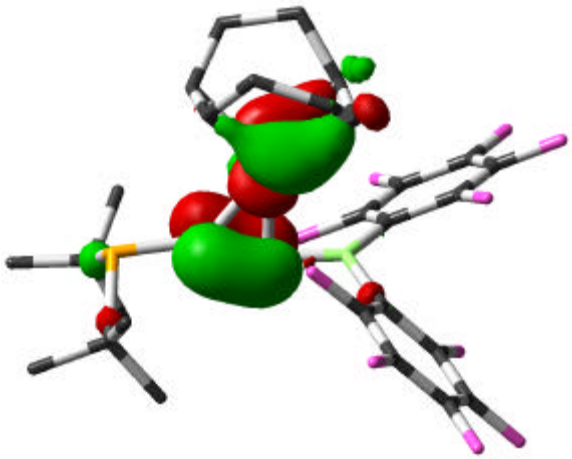

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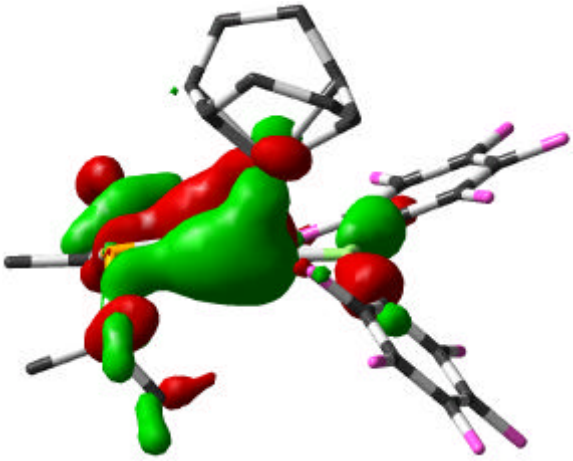

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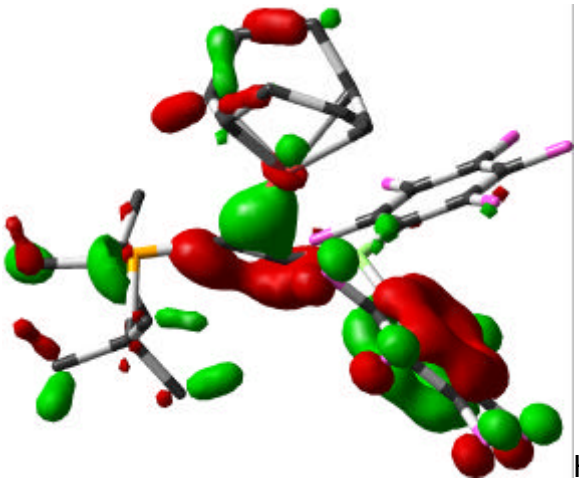

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Reference:

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